

Solution of the Boltzmann equation without the relaxation-time approximation

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A method is presented for solving the Boltzmann equation in layered systems without the relaxation-time approximation. The solution is compared with that obtained using the relaxation-time approximation for free-electron solids in the presence of boundaries. For the cases studied, most of the differences can be minimized by using the transport relaxation time. For nonfree electron materials it is expected that the differences will be more complex. [S0163-1829(99)05220-0]

I. INTRODUCTION

The relaxation-time approximation is almost universally used to simplify calculations of the conductivity. In multilayer systems, it has recently been used extensively to calculate (see Ref. 1 for reviews) the giant magnetoresistance,² which is the change in the electrical resistance that occurs in systems containing magnetic layers when the direction of magnetization is changed in some of the layers. For free-electron models, the resulting simplification allows analytic solutions when current flow is parallel to the interfaces.

A common approach for calculating the conductivity is to solve the semiclassical Boltzmann equation. A detailed discussion of the use of the Boltzmann equation in bulk systems is given by Allen.³ This approach has been applied to multilayer systems, using both free-electron⁴ and *ab initio* band structures.⁵ In most situations, solving the Boltzmann equation gives similar, if not identical, results to the other common approach, evaluating the Kubo formula (see Ref. 6 for a discussion of this issue for free electrons).

If the current is perpendicular to the interface, there is no analytic solution, even with the relaxation-time approximation. Recently, Zhang and Levy⁷ have examined the role of diffuse and specular interface scattering in this geometry, using the relaxation-time approximation. Valet and Fert⁸ used it to study the validity of a previously introduced macroscopic model. For this geometry a number of workers⁹ have studied the resistance due to a single barrier. The most detailed results were obtained by Kunze¹⁰ who obtained numerical results for the current and the particle density as well as for the barrier resistivity, again in the relaxation-time approximation. Schep *et al.*¹¹ have used a simplified model of bulk transport in conjunction with *ab initio* calculations of the transmission and reflection from ideal interfaces to compute the resistances of those interfaces.

There are two situations in which the relaxation-time approximation is exact. The first case is for isotropic scattering, which for free-electrons holds when the elastic impurity scattering is described by a delta function. In this case, the relaxation-time approximation remains exact in the presence of spatial variations. The second, more restrictive case occurs when the elastic impurity scattering depends only on the scattering angle, there is no spatial variation, and the trans-

port relaxation time (see Sec. II) is used for the relaxation time.

In this paper, we develop a method to solve the Boltzmann equation in layered systems without invoking the relaxation-time approximation. We then calculate the conductivity for several situations that involve free-electron metals with boundaries so that the systems are not homogeneous and the relaxation-time approximation is not strictly valid. The calculations are compared to those done using the relaxation-time approximation. The cases studied are (1) a single slab of finite thickness, diffuse reflection at the surfaces, and an applied electric field parallel to the surface and (2) an infinite free-electron metal divided by a partially reflecting interface with an applied field perpendicular to the interface. We find that the relaxation-time approximation describes the conductivity well as long as the relaxation time is chosen to be the transport relaxation time. It should be emphasized that in more anisotropic situations, such as *d*-band metals rather than free-electron metals, the relaxation-time approximation may not be adequate.

In Sec. II, we discuss the Boltzmann equation and the relaxation-time approximation for free-electron metals. In Sec. III, we examine the conductivity for the case of a thin slab, assuming a free-electron metal and nonspecular boundary scattering and in Sec. IV, the resistance at a partially reflecting interface is calculated for applied fields perpendicular to the interface. Section V is a summary of the paper. The formalism for solving the Boltzmann equation in layered systems is given in the Appendix.

II. THEORY

In this section, we first discuss the Boltzmann equation and the relaxation-time approximation, then we discuss the specific case of free-electron materials and impurity scattering that depends only on the scattering angle. The distribution function is given by $f(\mathbf{k}) = f_0(\epsilon_{\mathbf{k}}) + (\partial f_0 / \partial \epsilon)g(\mathbf{k})$ in the presence of an external field, where f_0 is the equilibrium distribution function. For metals, the changes in the distribution function can be restricted to energies close to the Fermi energy because the factor $\partial f_0 / \partial \epsilon$ is sharply peaked around the Fermi energy. For the linearized Boltzmann equation, the changes are approximated to occur only *on* the Fermi surface. The linearized Boltzmann equation for g is

$$v_z \frac{\partial g(\mathbf{k})}{\partial z} - \left[\frac{\partial g(\mathbf{k})}{\partial t} \right]_{coll} = eE v_{x,z}, \quad (1)$$

where $g(\mathbf{k})$ is the change in the electron distribution for wave vectors \mathbf{k} restricted to the Fermi surface. The change in the distribution arises from a field E assumed to be constant throughout the layer. The distribution also depends on spatial position, i.e., $g = g(\mathbf{k}, z)$, but this dependence of g on z will not be written explicitly. It is assumed that the geometry is such that the spatial dependence is only in the z direction; the system is uniform in the x and y directions. In Eq. (1) E is the external electric field and $v_{x,z}$ either is v_x or v_z depending on whether E is in the x or z direction, respectively. The velocities v_x or v_z are the x and z components of velocity at the Fermi surface.

The term that describes collisions with impurities is

$$- \left[\frac{\partial g(\mathbf{k})}{\partial t} \right]_{coll} = \frac{g(\mathbf{k})}{\tau_0(\mathbf{k})} - \int_{FS} d\mathbf{k}' P(\mathbf{k}, \mathbf{k}') g(\mathbf{k}'), \quad (2)$$

where the scattering relaxation time is

$$\frac{1}{\tau_0(\mathbf{k})} = \int_{FS} d\mathbf{k}' P(\mathbf{k}, \mathbf{k}'), \quad (3)$$

and $P(\mathbf{k}, \mathbf{k}')$ is the probability of scattering from \mathbf{k} to \mathbf{k}' . The first term on the right-hand side of Eq. (2), the scattering-out term, represents the rate that electrons are scattered out of the state \mathbf{k} . The second term, the scattering-in term, is the rate at which electrons are scattered into \mathbf{k} , $P(\mathbf{k}, \mathbf{k}')g(\mathbf{k}')$ being the rate at which electrons are scattered from \mathbf{k}' to \mathbf{k} . The isotropic part of g is not affected by collisions. For this part, the two terms on the right-hand side of Eq. (2) cancel each other. Only the anisotropic part of g relaxes.

The relaxation-time approximation replaces Eq. (2) with

$$- \left[\frac{\partial g(\mathbf{k})}{\partial t} \right]_{coll} = \frac{g(\mathbf{k}) - \bar{g}}{\tau(\mathbf{k})}, \quad (4)$$

where \bar{g} is the spatially dependent average of g over the Fermi surface.

$$\bar{g} = \frac{1}{4\pi} \int_{FS} d\mathbf{k} g(\mathbf{k}). \quad (5)$$

If the scattering is isotropic, the scattering probability can be factored out of the integral in the scattering-in term. Then, only the isotropic part of the distribution function remains. In this case, the relaxation-time approximation, Eq. (4), is exact. For a more general scattering function, the relaxation time in Eq. (4), τ , is allowed to be different from the scattering relaxation time τ_0 . Later in this section, we show that for free electrons with nonisotropic scattering, the transport relaxation time, defined below in Eq. (7), is a better approximation.

Up to this point the discussion has been general, (a) applicable to a nonfree-electron metal, and (b) no assumptions have been made about the dependence of P on \mathbf{k}, \mathbf{k}' . We now discuss the case of a free-electron metal; the general case is treated in the Appendix.

For the case of free electrons scattering elastically from spherically symmetric impurities, $P(\mathbf{k}, \mathbf{k}')$ is a function of the scattering angle $\theta_{\mathbf{k}, \mathbf{k}'}$ where $\cos(\theta_{\mathbf{k}, \mathbf{k}'}) = \hat{\Omega} \cdot \hat{\Omega}'$ and $\hat{\Omega} = \mathbf{k}/k_F$ is the direction of the momentum of an electron on the Fermi surface. In that case it can be shown that the *bulk* solution (no spatial variation) of Eq. (1) for $g(\hat{\Omega})$ is given by¹²

$$g(\hat{\Omega}) = \tau_{trans} eE v_F \cos(\theta), \quad (6)$$

for an electric field in the z direction, with $\cos(\theta) = \hat{\Omega} \cdot \hat{\mathbf{z}}$. The transport relaxation time is given by

$$\frac{1}{\tau_{trans}} = \int d\hat{\Omega}' P(\hat{\Omega}, \hat{\Omega}') (1 - \hat{\Omega} \cdot \hat{\Omega}'). \quad (7)$$

It is determined by $P(\hat{\Omega}, \hat{\Omega}') (1 - \hat{\Omega} \cdot \hat{\Omega}')$ rather than the differential scattering probability alone, $P(\hat{\Omega}, \hat{\Omega}')$, due to the scattering-in term of Eq. (2). τ_{trans} can be interpreted as the relaxation time for the momentum. A small angle electron scattering will not serve to randomize the electron momentum, thus the factor $(1 - \hat{\Omega} \cdot \hat{\Omega}')$ in Eq. (7) is small for small angle scattering. For isotropic scattering, these two times τ_0 and τ_{trans} are equal.

The Boltzmann equation in the relaxation-time approximation is

$$v_z \frac{\partial g(\hat{\Omega})}{\partial z} + \frac{g(\hat{\Omega}) - \bar{g}}{\tau(\hat{\Omega})} = eE v_{x,z}, \quad (8)$$

while the Boltzmann equation without the relaxation-time approximation is

$$v_z \frac{\partial g(\hat{\Omega})}{\partial z} + \frac{g(\hat{\Omega})}{\tau_0(\hat{\Omega})} - \int d\hat{\Omega}' P(\hat{\Omega}, \hat{\Omega}') g(\hat{\Omega}') = eE v_{x,z}, \quad (9)$$

where $\tau_0(\hat{\Omega})$ is given by Eq. (3). In the case of a delta function scattering potential, i.e., isotropic scattering, Eq. (9) reduces to Eq. (8), the Boltzmann equation in the relaxation-time approximation, with τ given by the scattering time τ_0 in Eq. (3).

III. THIN SLAB

We now calculate the conductivity of a slab in a free-electron model. The slab is confined to $-d/2 < z < d/2$ and is infinite in the x and y directions. The external field is taken to be in the x direction. The slab is shown in Fig. 2(a).

The Boltzmann equation is given by Eq. (9) with $v_{x,z} = v_x$. The change in the distribution function, $g(\hat{\Omega})$, is labeled g^+ or g^- depending on whether the component of velocity in the z direction, $v_F \cos(\theta)$, is in the positive or negative z direction. The boundary conditions are

$$\begin{aligned} g^+(\hat{\Omega}_{spec}) &= p_l g^-(\hat{\Omega}), & z &= -\frac{d}{2}, \\ g^-(\hat{\Omega}_{spec}) &= p_r g^+(\hat{\Omega}), & z &= \frac{d}{2}, \end{aligned} \quad (10)$$

where $\hat{\Omega}_{spec}$ denotes the direction of an electron that was traveling in a direction $\hat{\Omega}$ and is specularly reflected. The specularity coefficients p_l, p_r satisfy

$$0 \leq p_{l,r} \leq 1, \quad (11)$$

where $p=0$ denotes completely diffuse scattering and $p=1$ is the condition for completely specular scattering. It is easily verified by substitution that the solution of Eq. (8), the Boltzmann equation in the relaxation-time approximation, in this geometry is

$$\begin{aligned} g^+(\hat{\Omega}) &= (1 + F^+ e^{-(d+2z)/2\tau|v_z|}) e E v_x \tau, \\ g^-(\hat{\Omega}) &= (1 + F^- e^{(d+2z)/2\tau|v_z|}) e E v_x \tau, \end{aligned} \quad (12)$$

where $v_z = v_F \cos(\theta)$ and $v_x = v_F \sin(\theta) \cos(\phi)$. $e E v_x \tau$ is the bulk solution, Eq. (A11), i.e., the solution of the particular Eq. (A8), and the second term on the right-hand side of Eq. (12) is the solution of the homogeneous equation, Eq. (A6). The quantities F^+ and F^- are determined by substitution of Eq. (12) into Eq. (10). The conductivity per spin is then obtained from

$$\begin{aligned} \sigma_{\text{rta}} &= -\frac{e}{E} \frac{1}{(2\pi)^3} \frac{1}{d} \int_{-d/2}^{d/2} dz \int d^3k v_x g(\hat{\Omega}) \frac{\partial f_0}{\partial \epsilon} \\ &= -\frac{e}{E} \frac{1}{(2\pi)^3} \frac{m k_F}{\hbar^2} \frac{1}{d} \int_{-d/2}^{d/2} dz \int_{\text{FS}} d\hat{\Omega} v_x g(\hat{\Omega}) \end{aligned} \quad (13)$$

where $\mathbf{v} = (\hbar/m)\mathbf{k}$.

In the limit of specular reflection, $p_l = p_r = 1$, the slab mimics a bulk metal and the conductivity is given by the bulk value,

$$\sigma_0 = \frac{n e^2 \tau}{m}, \quad (14)$$

where n is the number of electrons (per spin) per unit volume, e is the electron charge, and m is the electron mass. Because we are interested in deviations from bulk behavior, we focus on the diffuse limit. For the case of purely diffuse scattering, $p_l, p_r = 0$, and $F^+ = -1$, $F^- = -e^{-d/\tau|v_z|}$. The conductivity for this case was first given by Sondheimer¹³ as

$$\frac{\sigma_{\text{relax}}}{\sigma_0} = 1 - \frac{3}{8s} + \frac{3}{2s} \int_1^\infty dt \left(\frac{1}{t^3} - \frac{1}{t^5} \right) e^{-st}, \quad (15)$$

where one has

$$s = \frac{d}{\tau v_F}. \quad (16)$$

The limiting forms of Eq. (15) are

$$\frac{\sigma_{\text{relax}}}{\sigma_0} = 1 - \frac{3}{8s}, \quad s \gg 1, \quad (17)$$

and

$$\frac{\sigma_{\text{relax}}}{\sigma_0} = \frac{3s}{4} \ln\left(\frac{1}{s}\right), \quad s \ll 1. \quad (18)$$

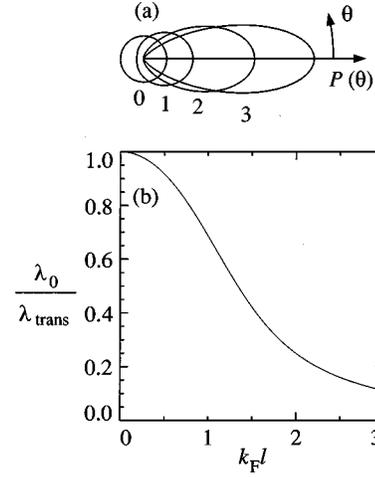


FIG. 1. Ratio of transport mean-free path to mean-free path. The inset (a) shows the anisotropy of the scattering probability, P , for indicated values of the parameter $k_F l = 0, 1, 2, 3$. The main panel (b) shows the corresponding ratios of the scattering time mean-free path to the transport mean-free path.

We choose a model for impurity scattering of the form

$$V(r) = A e^{-r^2/2l^2}, \quad (19)$$

where l is a parameter that measures the effective range of the potential and A is the strength. This model is chosen because it is simple and provides a length scale l for the scattering potential. In general, the defects that cause scattering are unknown, but should have a finite extent on the order of atomic dimensions. Below, we obtain numerical results for $k_F l = 0, 1, 2, 3$. In the limit that $l \rightarrow 0$, $V(r)$ is effectively a delta function so that $P(\hat{\Omega}, \hat{\Omega}')$ becomes constant and the relaxation-time approximation becomes valid. The scattering probability is given by

$$P(\hat{\Omega}, \hat{\Omega}') = \int d^3r e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}} V(\mathbf{r}), \quad (20)$$

in the Born approximation. Both \mathbf{k} and \mathbf{k}' lie on the Fermi surface. The model scattering potential is spherically symmetric so that P depends only on the angle between \mathbf{k} and \mathbf{k}' , the scattering angle $\theta_{\mathbf{k}, \mathbf{k}'}$. Use of Eq. (19) in Eq. (20) gives

$$P(\hat{\Omega}, \hat{\Omega}') = P(\theta_{\mathbf{k}, \mathbf{k}'}) = B e^{-(k_F l)^2 (1 - \cos \theta_{\mathbf{k}, \mathbf{k}'})}, \quad (21)$$

where k_F is the Fermi momentum. For a given $k_F l$, B determines the relaxation time. Figure 1(a) shows the anisotropy of the scattering probability P as the parameter $k_F l$ takes the values 0, 1, 2, 3.

Use of Eq. (21) in Eqs. (3) and (7) gives the ratio of the scattering time to the transport relaxation time, which is equal to the ratio of the scattering mean-free path λ_0 to the transport mean-free path

$$\frac{\tau_0}{\tau_{\text{trans}}} = \frac{\lambda_0}{\lambda_{\text{trans}}} = \frac{(e^{2a} - 2a - 1)}{(ae^{2a} - a)}, \quad (22)$$

where $a = (k_F l)^2$ (see Fig. 1). The transport mean-free path is given by

$$\lambda_{\text{trans}} = v_F \tau_{\text{trans}}, \quad (23)$$

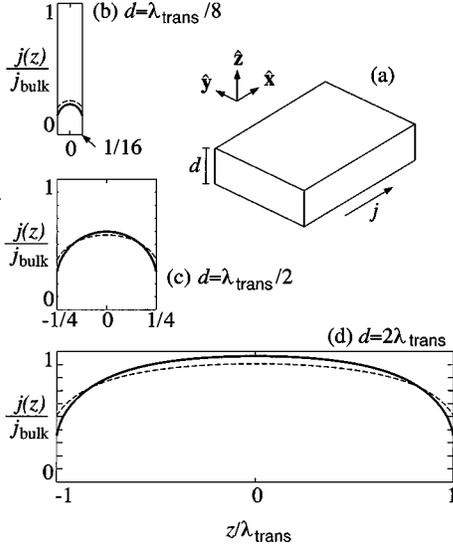


FIG. 2. Current distribution in a thin film. Panel (a) shows the geometry of thin slab indicating direction of current. Panels (c)–(d) show the exact current density (solid line) and current density calculated in the relaxation-time approximation (dashed line) for several values of the film thickness in terms of the transport mean-free path.

and we will take λ_{trans} to be the mean-free path when the relaxation-time approximation is used; $\tau \rightarrow \tau_{\text{trans}}$ and $v_F \tau \rightarrow \lambda_{\text{trans}}$.

The solution of the Boltzmann equation without the relaxation-time approximation is given in the Appendix. There, the distribution function is discretized onto a mesh of points \mathbf{k} on the Fermi surface, and the Boltzmann equation is solved on that mesh. For the thin film considered here, the solution on that mesh can be written

$$g^+_{\mathbf{k}} = \tau_{\text{trans}} e E v_{\mathbf{k}x} + \sum_{\lambda_i > 0} \xi_i e^{-\lambda_i z} x_{i,\mathbf{k}},$$

$$g^-_{\mathbf{k}} = \tau_{\text{trans}} e E v_{\mathbf{k}x} + \sum_{\lambda_i < 0} \xi_i e^{-\lambda_i z} x_{i,\mathbf{k}}, \quad (24)$$

where $g_{\mathbf{k}}$ is the value of g at a point \mathbf{k} on the Fermi surface. For a free-electron model, \mathbf{k} denotes a particular value of Ω . The superscript $+$ or $-$ refers to states moving in the positive or negative z direction, respectively. The first term is the driving term for the Boltzmann equation, the right-hand term in Eq. (1). The quantities \mathbf{x}_i and λ_i are the eigenvectors and eigenvalues, respectively, of the operator for a form of the scattering matrix [see Eqs. (A7), (A10), and (A14)]. The ξ_i are determined from the boundary conditions, Eq. (10). Electrons moving to the right must relax towards the bulk value of g as they move away from the left interface, hence the restriction $\lambda_i > 0$ in the first line of Eq. (24). The current density as a function of position is given by

$$j(z) = -e \frac{1}{(2\pi)^3} \frac{mk_F}{\hbar^2} \int_{\text{FS}} d\Omega v_x g(\Omega). \quad (25)$$

In practice, this is evaluated by a sum over the discrete mesh.

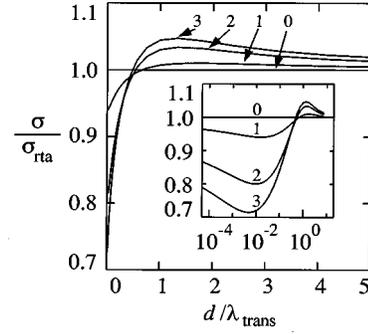


FIG. 3. Conductivity of a thin film. For the indicated values of $k_F l = 0, 1, 2, 3$, the main panel and the inset show the ratio of exact numerical conductivity to that calculated using the relaxation-time approximation as a function of the ratio of the film thickness to the transport relaxation-time mean-free path. The inset shows the region where the ratio d/λ_{rta} is very small.

We now assume purely diffuse scattering at the boundaries and we compare the current density calculated without the relaxation-time approximation to that calculated with the relaxation-time approximation (using the transport scattering time and mean-free path). The resulting current densities are shown in Fig. 2 for three different values of the film thickness; $d = \lambda_{\text{trans}}/8$, $\lambda_{\text{trans}}/2$, and $2\lambda_{\text{trans}}$. The results can be understood as follows. For the case shown in Fig. 2(b), $d = \lambda_{\text{trans}}/8$, the ‘‘exact’’ current is less than the relaxation-time approximation current for all values of z . Because of the diffuse scattering at the walls there are fewer electrons available there to scatter into a state Ω from some other state Ω' as can be seen from the second term on the right-hand side of Eq. (2). This means that the scattering time near the walls will be shorter than in the bulk and consequently the current will be smaller. The relaxation-time approximation is correct only for the uniform bulk situation and does not take proper account of the effects of the boundary conditions, e.g., $g^+ = 0$ at $z = -d/2$ [Eq. (10)], thus it over estimates the amount of scattering ‘‘in’’ from the second term on the right-hand side of Eq. (2). As the electrons move away from the wall they lose their memory of it on a length scale of the mean-free path. The exact solution has a shorter mean-free path near the walls and so it approaches the bulk current density at a faster rate than the relaxation-time approximation current, hence, the crossing of the currents in Fig. 2(c). Figure 2(d) is for a larger value of the slab width and shows the approach of the currents to the bulk value.

Figure 3 shows the ratio of the ‘‘exact’’ conductivity σ to that of the conductivity calculated in the relaxation-time approximation σ_{rta} again using the transport mean-free path λ_{trans} . This ratio is plotted versus d/λ_{trans} for various values of the parameter $k_F l$ in Eq. (21). For $k_F l = 0$, the scattering is isotropic, corresponding to a delta function scattering potential. As discussed earlier in the paper, the relaxation-time approximation is exact in this limit and the ratio of conductivities is unity. In the limit of large d/λ_{trans} , the electrons do not see the boundaries. In this isotropic situation the relaxation-time approximation is exact and the ratio of conductivities approaches one. For very small d/λ_{trans} , the ratio of conductivities behaves as shown in the insert of Fig. 3 and can be understood as follows. Equation (18) gives σ_{relax}

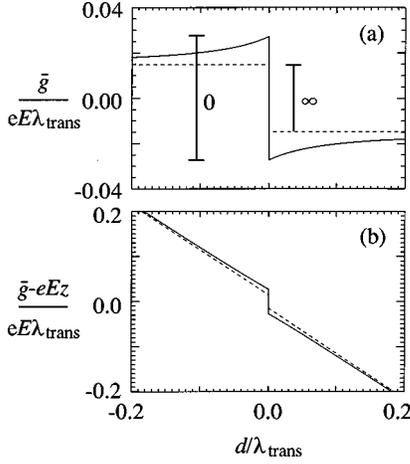


FIG. 4. Variation of chemical potential near an interface with a perpendicular current. The dashed lines indicate the chemical potentials far from the interface and the solid line includes the contribution of the exponential terms. In panels (a) and (b), the external electric field is, respectively, not included and included. The ∞ and 0 label the potential drop associated with the interface far from the interface and at the interface, respectively. The calculations use $k_{\text{F}l}=1$ and $n=8$ [see Eq. (28)].

$\sim d \ln(\lambda_{\text{trans}}/d)$. As described above, the relaxation-time approximation overestimates the mean-free path for electrons near a diffusely scattering boundary. If we assume the exact conductivity takes the form $d \ln(\lambda_{\text{eff}}/d)$ where $\lambda_{\text{eff}} < \lambda_{\text{trans}}$ then $\sigma/\sigma_{\text{rta}} \rightarrow 1$ as $d/\lambda_{\text{trans}} \rightarrow 0$ and $\sigma/\sigma_{\text{rta}}$ decreases as d/λ_{trans} increases from zero in agreement with the behavior shown in the inset of Fig. 3. However, there will be quantum effects in the region $d/\lambda_{\text{trans}} \ll 1$ that are not treated by the Boltzmann equation.

It is clear from the strong dependence of $\lambda_{\text{trans}}/\lambda_0$ on $k_{\text{F}l}$ shown in Fig. 1 that the good agreement between the “exact” conductivity and that calculated using the relaxation-time approximation depends on the use of the transport relaxation time.

IV. AN INFINITE METAL DIVIDED BY AN INTERFACE

We now consider the case of an infinite, free-electron metal divided by an interface at $z=0$. Electrons incident on the interface are reflected or transmitted with a probability that depends on their angle of incidence. For current perpendicular to the interface, the current density must be conserved and is thus constant, independent of z . Besides the resistivity due to impurity scattering there is an additional resistivity due to the fact that there will be only partial transmission across the interface. To force a finite current through the partially reflecting interface, it is necessary to build up a finite chemical potential difference across the interface. In general, the chemical potential will also have an exponential-like dependence on z that decays away from the interface on both sides. Figure 4 shows the behavior of the chemical potential near the interface. In Fig. 4(a) the variation due to the external field is not included and in Fig. 4(b) it is. In both panels, the dashed lines show the extrapolation of the chemical potential difference far from the interface back to the interface, this difference is labeled ∞ in the figure. The

chemical potential difference at the interface is labeled 0. Charge neutrality is imposed by identifying $g - \bar{g}$ as the electron distribution and $-\partial g/\partial z$ as the additional electric field required to maintain neutrality. The interface resistivity is given by the ratio of the extrapolated chemical potential difference divided by the current through the interface.

In this geometry, the relaxation-time approximation to the Boltzmann equation cannot be solved analytically as can be done when the current is parallel to the barrier. The Boltzmann equation is given by

$$v_z \frac{\partial g_i(\Omega)}{\partial z} + \frac{g_i(\Omega)}{\tau_0(\Omega)} - \int d\Omega' P(\Omega, \Omega') g_i(\Omega') = e E v_z, \quad (26)$$

where $i=1,2$ denotes the metal to the left or right of $z=0$, respectively. The scattering probability is given by Eq. (21). As previously, the change in the distribution function $g_i(\Omega)$ will be labeled g^+ or g^- depending on whether the component of velocity in the z direction, $v_{\text{F}} \cos(\theta)$, is in the positive or negative z direction. The boundary conditions at $z=0$ are

$$\begin{aligned} g_1^- &= R_{11} g_1^+ + T_{12} g_2^-, \\ g_2^+ &= R_{22} g_2^- + T_{21} g_1^+, \end{aligned} \quad (27)$$

where R_{ii} is the probability that an electron in region i , is reflected back into i and T_{ij} is the probability that the electron is transmitted from region j into region i . The reflection and transmission coefficients are modeled as

$$R_{ii}(\theta) = 1 - T_{ij}(\theta) = \frac{\alpha}{\alpha + \cos^n(\theta)}, \quad (28)$$

where θ is the angle of incidence and α and n are parameters. This form is a generalization of the result¹⁴ for a sheet delta function potential of strength $\hbar v_{\text{F}} \sqrt{\alpha}$ at $z=0$, for which $n=2$. A sheet delta function with an appropriate amplitude is a good approximation for the low-energy reflection from planar defects, like stacking faults, where the electronic structure is the same on both sides of the interface.¹⁵ For interfaces between dissimilar materials, reflection is more complicated. To examine a range of behaviors while maintaining a simple form for the reflection, we generalize the exponent n to other values.

The boundary conditions require g_i to not diverge far from the interface, thus the solution given by Eq. (A20) and Eq. (A11) takes the form

$$\begin{aligned} g_{1\mathbf{k}} &= \tau_{\text{trans}} e E v_{\mathbf{k}z} + \xi_0^{(1)} z_{\mathbf{k}} + \xi_1^{(1)} (z_{\mathbf{k}z} - z_{\mathbf{k}}') \\ &+ \sum_{\lambda_i < 0} \xi_i^{(1)} e^{-\lambda_i z} x_{i,\mathbf{k}}, \\ g_{2\mathbf{k}} &= \tau_{\text{trans}} e E v_{\mathbf{k}z} + \xi_0^{(2)} z_{\mathbf{k}} + \xi_1^{(2)} (z_{\mathbf{k}z} - z_{\mathbf{k}}') \\ &+ \sum_{\lambda_i > 0} \xi_i^{(2)} e^{-\lambda_i z} x_{i,\mathbf{k}}, \end{aligned} \quad (29)$$

in regions 1 and 2. The first term on the right-hand side of Eq. (29) is the bulk solution in layer i for field E_i . The second term represents a uniform shift in the Fermi energy

because $z_{\mathbf{k}}=1$ and $f=f_0+(\partial f_0/\partial \epsilon)g$. The third term is given by Eq. (A16) and it is clear from Eq. (A19) that unlike the second term, it carries current. If the correct value of E_i is used in the first term, then $\xi_1^{(i)}=0$, otherwise this term essentially corrects the field and the associated current flow. The exponential terms do not carry current perpendicular to the interface because current conservation is incompatible with an exponential variation.

The interface resistance, R , is given by the relation $\Delta V=IR$ where $\Delta V=(\xi_0^{(1)}-\xi_0^{(2)})/e$ is the potential drop across the interface and $I=jA$ where j is the current density through the interface and A is the cross sectional area of the interface. The interface resistance, R , is the additional resistance of the sample due to the interface. It is useful to define an additional resistance R_0 to be the total potential drop at the interface divided by the current. It is obtained by replacing $\xi_0^{(i)}$ above by $\xi_0^{(i)}+\delta\mu_{\text{exp},i}(z=0)$. $\delta\mu_{\text{exp},i}(z=0)$ is the change in the Fermi energy at the interface in region $i=1,2$ due to the exponential terms in Eq. (29) and it is given by the Fermi surface average of those terms evaluated at $z=0$.

The current density is

$$j(z)=-e\frac{1}{(2\pi)^3}\frac{mk_{\text{F}}}{\hbar^2}\int_{\text{FS}}d\hat{\Omega}v_zg(\hat{\Omega}), \quad (30)$$

and is constant throughout the metal.

The discretization of $\hat{\Omega}$ is such that $\hat{\Omega}_{\mathbf{k}}$ takes on N values in each region so the boundary conditions Eq. (27) constitute N equations. There are $N/2-1$ values of $\xi_i^{(1)}$ and $N/2-1$ values of $\xi_i^{(2)}$ in Eq. (29) as well as $\xi_0^{(1)}$, $\xi_0^{(2)}$, $\xi_1^{(1)}$, and $\xi_1^{(2)}$. We choose $\xi_0^{(1)}=-\xi_0^{(2)}=\xi_0$, which corresponds to a relative shift in the Fermi energies in regions 1 and 2 corresponding to a potential difference between the two regions created by the applied field. As discussed above, $\xi_1^{(2)}=\xi_1^{(1)}=0$, because the current density is equal to its bulk value everywhere. With these choices we can find $g_{1\mathbf{k}}, g_{2\mathbf{k}}$ and calculate the interface resistance, R , as well as the resistance at the interface, R_0 .

The term $\mathbf{z}\mathbf{z}-\mathbf{z}'\mathbf{z}'$ [see Eq. (A16)] can be understood as an electrochemical potential (the gradient of which gives a field) and an associated current flow. In the general case of perpendicular transport, the bulk conductivities will differ from layer to layer, so the internal fields will be different from layer to layer. One way to solve for the overall conductivity is to impose a bulk-current density at infinity, and then solve the boundary conditions from layer to layer to determine the internal fields. In this approach, the solution $\mathbf{z}\mathbf{z}-\mathbf{z}'\mathbf{z}'$ plays a crucial role in each layer. An alternate approach is to solve the particular equation in each layer and find the field that is necessary to make the current the same in each layer. In this approach, the solution $\mathbf{z}\mathbf{z}-\mathbf{z}'\mathbf{z}'$ plays no role, because it has already been accounted for by the particular solution and the field. We have used this latter approach in the work described here. The relationship between $\mathbf{z}\mathbf{z}-\mathbf{z}'\mathbf{z}'$, the field E , and the particular solution is given by Eq. (A19).

The behavior of the interface resistance can be understood in greater detail by examining the current density and ‘‘chemical potential’’ as a function of position on the Fermi surface. It is useful to define

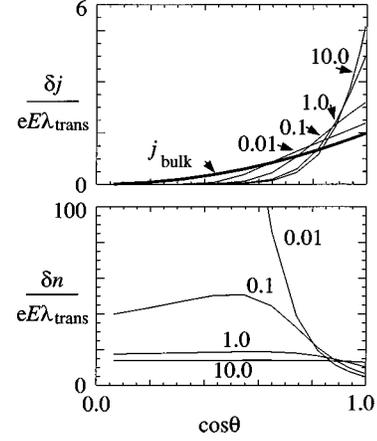


FIG. 5. Angular dependence of current through an interface. Panel (a) shows the current density, Eq. (32), for various values of α as a function of $\cos(\theta)$. Panel (b) shows the ‘‘chemical potential’’ $\delta\mu$, Eq. (33), for various values of α as a function of $\cos(\theta)$. The calculations use $k_{\text{F}l}=1$ and $n=8$.

$$\delta\mu=(g_2^++g_2^-)-(g_1^++g_1^-), \quad (31)$$

where g_i^+ refers to an electron moving to the right in the direction $\hat{\Omega}$ and g_i^- refers to an electron moving in a direction corresponding to specular scattering at the interface, i.e., $\theta\rightarrow(\pi-\theta)$ and $\phi\rightarrow\phi$. The quantities g_i^\pm correspond to the same value of momentum parallel to the interface. We also define

$$\delta j=(g_i^+-g_i^-)\cos(\theta), \quad (32)$$

where conservation of current requires δj to be independent of i for interfaces with no diffuse scattering, as we consider here.

Combining Eqs. (27), (28), (31), and (32) gives

$$\delta\mu=-2\alpha\delta j/\cos^{n+1}\theta, \quad (33)$$

which can be solved by $\delta\mu\propto\alpha$ and $\delta j\propto\cos^{n+1}\theta$. We find that this solution holds in the limit that $\alpha\rightarrow\infty$, where strong reflection for all angles gives a large $\delta\mu$ only weakly dependent on angle. From Eq. (29), it is clear that δj depends on the ξ_i terms, the coefficients of the exponentially varying terms, and not on ξ_0 , while $\delta\mu$ depends on both the ξ_i and ξ_0 . We conclude that for large α , $\xi_0\propto\alpha$ while the ξ_i are roughly independent of α . Since the exponential terms depend strongly on θ , δj has a strong angular variation in this limit. This behavior for large α is illustrated in Fig. 5 for values of α corresponding to strong reflection. For small α , on the other hand, the reflection is weak near the zone center, $\cos(\theta)\sim 1$, and the current distribution is very close to the bulk distribution, $\cos^2(\theta)$. This, in turn leads to a strong dependence of $\delta\mu$ on θ . The consequences of the limiting behaviors of α behavior are shown in Figs. 6 and 7.

As a function of α , Figs. 6(a) and 7(a) show the interface resistance R_{ita} , the resistance calculated using the relaxation-time approximation to the Boltzmann equation, Eq. (8), and the transport lifetime. The linear dependence of R_{ita} on α is a direct result of the fact that the interface resistance, R , is given by the relation $\Delta V=IR$ where $\Delta V=(\xi_0^{(1)}-\xi_0^{(2)})/e$ and $\xi_0\sim\alpha$.

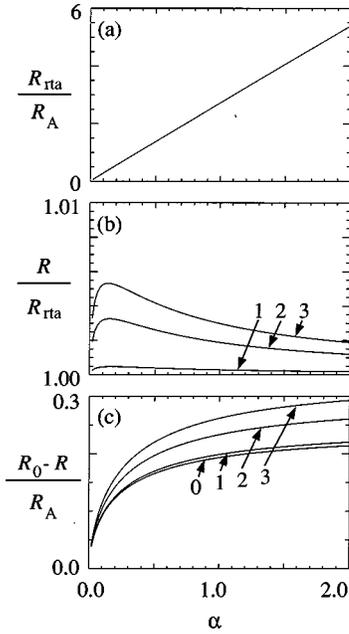


FIG. 6. Interface resistance as a function of reflection strength. Panel (a) shows the interface resistance calculated in the relaxation-time approximation with the transport lifetime versus α for $n=2$, see Eq. (28). The resistance is scaled by $R_A = 6\pi m / (Ae^2 k_F^3)$. Panel (b) shows the ratio of the exact barrier resistance to that calculated in the relaxation-time approximation with the transport lifetime for $k_F l = 1, 2, 3$. Panel (c) shows the difference between the interface resistance R related to the potential drop in Fig. 4(a) labeled ∞ and that labeled 0.

Figures 6(b) and 7(b) are plots of the ratio R/R_{rta} . The curves are for the values $k_F l = 0, 1, 2, 3$. The relaxation-time approximation to the Boltzmann equation using the transport lifetime corresponds to $k_F l = 0$. The independence of R/R_{rta} on α also follows from the linear dependence of ξ_0 on α .

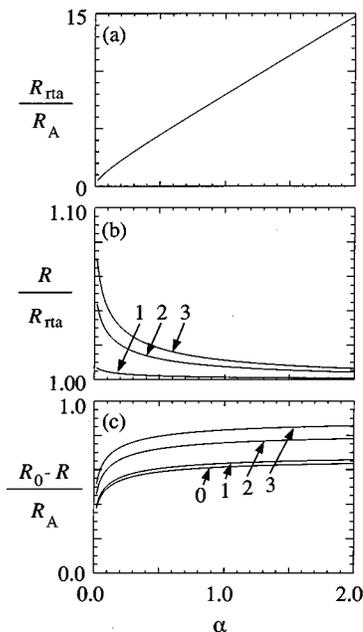


FIG. 7. Interface resistance as a function of reflection strength. Same as Fig. 6, but for $n=8$.

The fact that $R/R_{\text{rta}} \rightarrow 1$ implies that the exponential terms become constant, independent of α , for large α .

Figures 6(c) and 7(c) show the interface resistance difference, $R - R_0$, versus α for $k_F l = 0, 1, 2, 3$. The difference, $R - R_0$, depends only on the exponential terms which do not depend on α for large α , hence, the saturation of the curves.

The case $n=1$ is a special case where there is no exponential contribution to the charge density, the terms on the right-hand side of Eq. (29) vanish. In that case the interface resistance is given by

$$R = 2\alpha \frac{6\pi^2 m}{Ae^2 k_F^3} = 2\alpha R_A. \quad (34)$$

This quantity is identical to the resistance that describes the total potential drop across the interface, and there are no corrections to the relaxation-time approximation.

V. SUMMARY

A method is presented for solving the spatially varying Boltzmann equation without the making the relaxation-time approximation. This method is presented in the Appendix and involves a discretization of points on the Fermi surface. The scattering terms can then be inverted by matrix methods and the spatial part of the equation can be dealt with analytically.

The solution is compared with that obtained using the relaxation-time approximation for free-electron solids in the presence of boundaries. The cases studied are (a) a single slab of finite thickness with nonspecular reflection at the surfaces and an applied electric field parallel to the surface and (b) the case of an infinite free-electron metal divided by a partially reflecting interface with an applied field. For the cases studied, most of the differences can be minimized by using the transport relaxation time. For reasonable values of the parameters maximum differences in conductivities or resistances are of order 10% and typically the differences are considerably smaller. For nonfree-electron materials it is expected that the differences will be more complex because the transport relaxation time is exact only for an isotropic bulk material.

ACKNOWLEDGMENTS

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APPENDIX

In a homogeneous layer, the linearized Boltzmann equation to be solved is, from Eqs. (1) and (2),

$$v_z \frac{\partial g(\mathbf{k})}{\partial z} + \frac{g(\mathbf{k})}{\tau_0(\mathbf{k})} - \int_{\text{FS}} d\mathbf{k}' P(\mathbf{k}, \mathbf{k}') g(\mathbf{k}') = A(\mathbf{k}), \quad (A1)$$

where $A(\mathbf{k})$ is the term due to the external electric field. The solutions from several layers can be joined together using the boundary conditions between the layers to give the result for a composite structure. In order to solve Eq. (A1) we discretize it

$$v_{zk} \frac{\partial g_{\mathbf{k}}}{\partial z} + \frac{g_{\mathbf{k}}}{\tau_{\mathbf{k}}} - \sum_{\mathbf{k}'} \Delta_{\mathbf{k}'} P_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}'} = A_{\mathbf{k}}, \quad (\text{A2})$$

where $g_{\mathbf{k}}$ is the value of g at a point \mathbf{k} on the Fermi surface and $\Delta_{\mathbf{k}}$ is a weighting factor such that

$$\sum_{\mathbf{k}} \Delta_{\mathbf{k}} = \int d\Omega, \quad (\text{A3})$$

and

$$\frac{1}{\tau_{\mathbf{k}}} = \sum_{\mathbf{k}'} \Delta_{\mathbf{k}'} P_{\mathbf{k},\mathbf{k}'}, \quad (\text{A4})$$

where $P_{\mathbf{k},\mathbf{k}'}$ is symmetric.

The spatial dependence of Eq. (A2) can be solved by finding the solutions to the particular and to the homogeneous equations. The particular equation is

$$\frac{g_{\mathbf{k}}}{\tau_{\mathbf{k}}} - \sum_{\mathbf{k}'} \Delta_{\mathbf{k}'} P_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}'} = A_{\mathbf{k}}, \quad (\text{A5})$$

while the homogeneous equation is

$$v_{zk} \frac{\partial g_{\mathbf{k}}}{\partial z} + \frac{g_{\mathbf{k}}}{\tau_{\mathbf{k}}} - \sum_{\mathbf{k}'} \Delta_{\mathbf{k}'} P_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}'} = 0. \quad (\text{A6})$$

It is useful to define

$$B_{\mathbf{k},\mathbf{k}'} = \frac{\delta_{\mathbf{k},\mathbf{k}'}}{\tau_{\mathbf{k}}} - \Delta_{\mathbf{k}'} P_{\mathbf{k},\mathbf{k}'}, \quad (\text{A7})$$

so that the particular equation, Eq. (A5), becomes

$$\sum_{\mathbf{k}'} B_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}'} = A_{\mathbf{k}}, \quad (\text{A8})$$

and the homogeneous equation, Eq. (A6), is written as

$$\sum_{\mathbf{k}'} \left(\delta_{\mathbf{k},\mathbf{k}'} \frac{\partial}{\partial z} + [V^{-1}B]_{\mathbf{k},\mathbf{k}'} \right) g_{\mathbf{k}'} = 0, \quad (\text{A9})$$

where one has

$$V_{\mathbf{k},\mathbf{k}'} = v_{zk} \delta_{\mathbf{k},\mathbf{k}'}. \quad (\text{A10})$$

The matrices B and $V^{-1}B$ are both asymmetric and singular, since $\sum_{\mathbf{k}'} B_{\mathbf{k},\mathbf{k}'} = 0$.

For the free-electron case when P depends only on scattering angle, the solution of Eq. (A8) is given by Eq. (6), which in the notation of this appendix is

$$g_{\mathbf{k}} = \tau_{\text{trans}} A_{\mathbf{k}}, \quad (\text{A11})$$

where τ_{trans} is given by Eq. (7).

In general, Eq. (A5) has the formal solution

$$g_{\mathbf{k}} = \sum_{\mathbf{k}'} B_{\mathbf{k},\mathbf{k}'}^{-1} A_{\mathbf{k}'}, \quad (\text{A12})$$

but the matrix $B_{\mathbf{k},\mathbf{k}'}$ is singular. The eigenvector \mathbf{z} , corresponding to the zero eigenvalue of B has constant components, $z_{\mathbf{k}} = 1$, because

$$(B\mathbf{z})_{\mathbf{k}} = \sum_{\mathbf{k}'} B_{\mathbf{k},\mathbf{k}'} z_{\mathbf{k}'} = \sum_{\mathbf{k}'} B_{\mathbf{k},\mathbf{k}'} = 0. \quad (\text{A13})$$

If Eq. (A6) is satisfied by a g then $g + \text{constant} \times \mathbf{z}$ is also a solution. The solutions of Eq. (A12) for $g_{\mathbf{k}}$ that are of physical interest can be obtained numerically from the singular value decomposition of B . The numerical solution we use gives a result that is orthogonal to \mathbf{z}^T . For the free-electron case, when P depends only on scattering angle, the first term on the right-hand side of Eq. (A20) is given by $\tau_{\text{trans}} A_{\mathbf{k}}$.

The homogeneous equation, Eq. (A9), can be solved as follows. Denote the right eigenvectors of $V^{-1}B$ by \mathbf{x}_i and the corresponding eigenvalues by λ_i where

$$V^{-1}B\mathbf{x}_i = \lambda_i \mathbf{x}_i. \quad (\text{A14})$$

Then the expression

$$g = \sum_i \xi_i e^{-\lambda_i z} \mathbf{x}_i, \quad (\text{A15})$$

is seen to be a solution of Eq. (A9) by substitution. The ξ_i are constants to be determined by the boundary conditions.

A complication is that, for $V^{-1}B$, the zero eigenvalue is doubly degenerate with the same eigenvector \mathbf{z} , as discussed above. The matrix is referred to as defective and is said to have a nontrivial Jordan block. Consequently, the two terms that correspond to zero eigenvalues, $\lambda_i = 0$, are not included in Eq. (A15) because they have a different form. The constant term $\xi_0 \mathbf{z}$ is one additional term in the solution. Because the eigenvalue is degenerate there is another solution of the homogeneous equation, Eq. (A9),

$$\xi_1 (z\mathbf{z} - \mathbf{z}'), \quad (\text{A16})$$

where one has

$$\mathbf{z}' = B^{-1}V\mathbf{z}. \quad (\text{A17})$$

The fact that $z\mathbf{z} - \mathbf{z}'$ is a solution of Eq. (A9) can be verified by substitution. We note that \mathbf{z}' is only defined to within an additional term proportional to \mathbf{z} . The numerical procedure we use to obtain \mathbf{z}' gives a result that is orthogonal to \mathbf{z}^T .

When the electric field is in the x direction, which is translationally invariant, the term $z\mathbf{z} - \mathbf{z}'$ does not play a role, because there is no current flow in the z direction and the coefficient of \mathbf{z}' must be zero, so the term is discarded. However, in the case that the electric field is in the z direction, $z\mathbf{z} - \mathbf{z}'$ is an essential part of the solution for g . In that case Eq. (10), the solution for the bulk value of g becomes

$$g_{\text{bulk}} = B^{-1}eEv_z = eEB^{-1}V\mathbf{z}. \quad (\text{A18})$$

Comparison with Eq. (A17) gives

$$g_{\text{bulk}} = eE\mathbf{z}'. \quad (\text{A19})$$

Thus, \mathbf{z}' is proportional to g_{bulk} and the second term on the right-hand side of Eq. (A16) is one that carries current. The linear z -dependent portion of $z\mathbf{z} - \mathbf{z}'$, which can be interpreted either as a chemical potential gradient or an external field, implies the current carrying part \mathbf{z}' .

From Eqs. (A12), (A15), and the discussion following Eq. (A15), our final result is

$$g_{\mathbf{k}} = \sum_{\mathbf{k}'} B_{\mathbf{k},\mathbf{k}'}^{-1} A_{\mathbf{k}'} + \xi_0 z_{\mathbf{k}} + \xi_1 (z_{\mathbf{k}z} - z'_{\mathbf{k}}) + \sum_i' \xi_i e^{-\lambda_i z} x_{i,\mathbf{k}}, \quad (\text{A20})$$

where the λ_i are given by Eq. (A14) and the ξ are to be determined by the boundary conditions. The two values of i for which $\lambda_i=0$ are excluded from the summation in Eq. (A20). If the correct field E is used to find the particular solution, the first term in Eq. (A20), then ξ_1 will be zero. Otherwise, the term $\xi_1(z_{\mathbf{k}z} - z'_{\mathbf{k}})$ will compensate to give the correct field and current.

The particular solution and the two terms associated with zero eigenvalues control the current and the constant part of the field in each layer. The exponential terms also have an isotropic part and contribute to the variation of the field, but they do not carry current perpendicular to the interface. Only the particular solution and the $\xi_1(z_{\mathbf{k}z} - z'_{\mathbf{k}})$ terms carry current in that direction. While the exponential terms do not carry current, they do change the angular distribution of the current. This redistribution is why these terms are important near interfaces. They change the angular dependence of current distribution from that of the bulk to that which gets through the interface.

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